

The CP-PACS Project and Lattice QCD Results

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(Received)

The aim of the CP-PACS project was to develop a massively parallel computer for performing numerical research in computational physics with primary emphasis on lattice QCD. The CP-PACS computer with a peak speed of 614 GFLOPS with 2048 processors was completed in September 1996, and has been in full operation since October 1996. We present an overview of the CP-PACS project and describe characteristics of the CP-PACS computer. The CP-PACS has been mainly used for hadron spectroscopy studies in lattice QCD. Main results in lattice QCD simulations are given.

§1. Introduction

Lattice QCD is a fundamental theory of quarks and gluons which are constituents of hadrons such as protons and pions. Numerical studies of lattice QCD have developed significantly during the past decade in parallel with the development of computers. Of particular importance in this regard has been the construction of dedicated QCD computers (see for reviews Ref.1)) and the move of commercial vendors toward parallel computers in recent years. In Japan the first dedicated QCD computer was developed in the QCDPAX project²⁾. The QCDPAX computer with a peak speed of 14GFLOPS is actually the 5th computer in the PAX project³⁾, which pioneered the development of parallel computers for scientific and engineering applications in Japan.

The CP-PACS project was conceived as a successor of the QCDPAX project in the early summer of 1991. The project name CP-PACS is an acronym for Computational Physics by a Parallel Array Computer System. The aim of the project was to develop a massively parallel computer for carrying out research in computational physics with primary emphasis on lattice QCD.

In this article after a brief description of lattice QCD and the background of the project in Sec.2, we present an overview of the CP-PACS project in Sec.3, and describe characteristics of the CP-PACS computer in Sec.4. The performance of the computer for lattice QCD applications as well as for the LINPACK benchmark are also given. Main results in lattice QCD are given in Sec.5. Sec.6 is devoted to conclusions.

§2. Lattice QCD and Background of the Project

Lattice QCD is a fundamental theory of quarks and gluons defined in terms of the path-integral formalism of quantum theory on a 4-dimensional hyper-cubic

lattice. The lattice spacing plays a role of an ultra-violet cutoff. The infinite volume limit and the continuum limit should be taken in order to get physical quantities.

As we have to treat quarks and gluons relativistically, we have a problem in 4-dimension instead of 3-dimension as in solid-state problems. However, except this difference of dimensionality, it is a statistical system. Quarks are defined on sites, while gluons on bonds of a 4-dimensional hyper-cubic lattice. Numerical methods we employ are a Monte Carlo method, a molecular dynamics and a hybrid method of combination of these methods. However, due to this dimensionality, we need a lot of CPU time and a large memory size.

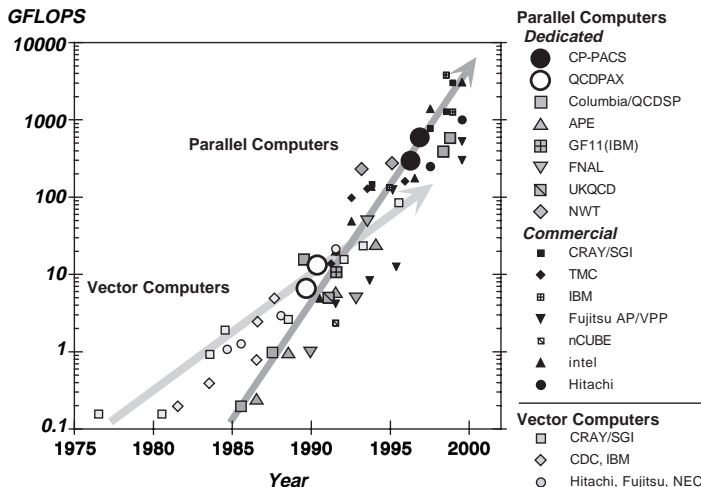


Fig. 1. Recent development of computers in term of theoretical peak speed.

Because of this requirement of high performance computers for numerical simulations in lattice QCD, dedicated machines have been constructed in USA, Europe and Japan. There are two additional reasons why dedicated parallel computers were widely developed for lattice QCD: First there is an incentive to perform first-principle calculations without introducing any approximations based on the fundamental law. Second there is a spiritual atmosphere in high-energy physics community to construct a special purposed equipment like an accelerator. A massively parallel computer is an accelerator for numerical simulations.

Fig. 1 shows the recent development of the computers in terms of the theoretical peak speed versus the year when the computer was shipped or constructed. Small open symbols are for vector-type supercomputers, while large and small filled symbols are for dedicated parallel and commercial parallel computers, respectively. Open circles with dot are for QCDPAX and filled large circles are for CP-PACS. We clearly observe that the rate of the progress for parallel computers is roughly double that of vector computer and that a crossover in the peak speed took place from vector to parallel computers around 1991. For this development dedicated machines for lattice QCD made important roles.

Table I. CP-PACS Project members

hardware	software	particle physics	astrophysics	condensed matter
K. Nakazawa ^a	I. Nakata ^e	Y. Iwasaki ^c	S. Miyama ^o	S. Miyashita ^p
H. Nakamura ^b	Y. Yamashita ^e	A. Ukawa ^k	T. Nakamura ^l	M. Imada ^q
T. Boku ^c	Y. Oyanagi ^f	K. Kanaya ^c	M. Umemura ^c	K. Nemoto ^r
T. Hoshino ^d	T. Kawai ^g	S. Aoki ^k	Y. Nakamoto ^c	A. Oshiyama ^k
T. Shirakawa ^d	M. Mori ^h	T. Yoshie ^c		S. Gunji ^c
K. Wada ^e	Y. Watase ⁱ	M. Okawa ^l		
M. Yasunaga ^e	S. Ichii ^j	N. Ishizuka ^c		
S. Sakai ^c		M. Fukugita ^m		
		H. Kawai ⁿ		

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ⁿ Theory Division, KEK

^o National Astronomical Observatory

^p Department of Physics, Osaka University

^q Institute of Solid State Physics, University of Tokyo

^r Department of Physics, Hokkaido University

§3. CP-PACS Project

The CP-PACS Project⁴⁾ aimed at developing a massively parallel computer designed to achieve high performance for numerical research of the major problems of computational physics, and it further aimed at significant progress in the solution of these problems through the application of the parallel computer upon completion of its development.

The Project formally started in April of 1992, and continued for five years, until March of 1997. The Project received about 2.2 billion Yen spread over the five year period. The Center for Computational Physics was founded in April 1992 at University of Tsukuba to carry out the Project, as well as to promote research in computational physics and parallel computer science. The Center is an inter-university facility open to researchers in academic institutions in Japan.

The Project members consist of 15 computer scientists and 18 physicists, as listed in Table I. As Table I clearly shows, the CP-PACS Project is a multi-disciplinary effort toward the advancement of computational physics encompassing not only several branches of physics but also computer science to develop parallel computers best suited for such applications. The Project was headed by Y. Iwasaki. The development of the CP-PACS computer was led by K. Nakazawa.

A unique feature of the Project is its emphasis on cross-disciplinary research involving both physicists and computer scientists. This is a tradition carried over from the QCDPAX Project²⁾, which is the predecessor and stepping stone for the CP-PACS Project. A close collaboration of researchers from the two disciplines has been both important and fruitful in reaching a design for the CP-PACS computer which best balances the computational needs of physics applications with the latest of computer technologies.

Development of a massively parallel computer requires advanced semiconductor technology. We selected Hitachi Ltd. as the industrial partner through a formal bidding process in the early summer of 1992, and we worked in a close collaboration for the hardware and software development of the CP-PACS computer. The first stage of the CP-PACS computer consisting of 1024 processing units with a peak speed of 307 GFLOPS was completed in March 1996. An upgrade to a 2048 system with a peak speed of 614GFLOPS was completed at the end of September 1996

§4. CP-PACS Computer

4.1. Architecture

The CP-PACS computer is an MIMD (Multiple Instruction-streams Multiple Data-streams) parallel computer with a theoretical peak speed of 614GFLOPS and a distributed memory of 128 Gbytes. The system consists of 2048 processing units (PU's) for parallel floating point processing and 128 I/O units (IOU's) for distributed input/output processing. These units are connected in an $8 \times 17 \times 16$ three-dimensional array by a three-dimensional crossbar network. The specification of the CP-PACS computer is summarized in Table II. A well-balanced performance of CPU, network and I/O devices supports the high capability of CP-PACS for massively parallel processing.

The basic strategy we adopted for the design is the usage of a fast RISC micro-processor for high arithmetic performance at each node and a linking of nodes with a flexible network so as to be able to handle a wide variety of problems in computational physics. The unique features of the CP-PACS computer reflecting these goals are represented by the special node processor architecture called *pseudo vector processor based on slide-windowed registers (PVP-SW)*⁵⁾ and the choice of a three-dimensional crossbar network.

4.2. Node processor

Each PU of the CP-PACS has a custom-made superscalar RISC processor with an architecture based on PA-RISC 1.1. In large scale computations in scientific and engineering applications on a RISC processor, the performance degradation occurring when the data size exceeds the cache memory capacity is a serious problem. For the processor of CP-PACS, an enhancement of the architecture called the PVP-SW⁵⁾ was developed to resolve this problem, while still maintaining upward compatibility with the PA-RISC architecture.

Table II. Specification of the CP-PACS computer

peak speed	614Gflops(64 bit data)
main memory	128GB
parallel architecture	MIMD with distributed memory
number of nodes	2048
node processor	HP PA-RISC1.1+PVP-SW
#FP registers	128
clock cycle	150MHz
1st level cache	16KB(I)+16KB(D)
2nd level cache	512KB(I)+512KB(D)
network	3-d crossbar
node array	$8 \times 17 \times 16^*$
through-put	300MB/sec
latency	$2.5 \sim 3.1 \mu\text{sec}$
distributed disks	3.5" RAID-5 disk
total capacity	595GB
software	
OS	UNIX, micro kernel
language	FORTRAN, C, assembler
Size	7.0m(width) \times 4.2m(depth) \times 2.0m(hight)
Power dissipation	275 KW maximum

*including nodes for disk I/O

4.3. Network

The 2048 processors are arranged in a three-dimensional $8 \times 16 \times 16$ array. The Hyper Crossbar network is made of crossbar switches in the x, y and z directions, connected together by an Exchanger at each of the three-dimensional crossing points of the crossbar array. Each exchanger is connected to a PU or IOU. Thus any pattern of data transfer can be performed with the use of at most three crossbar switches. Since the network has a huge switching capacity due to the large number of crossbar switches, the sustained data transfer throughput in general applications is very high.

4.4. Performance

The most CPU consuming part of lattice QCD calculations is the inversion of a linear equation. We developed a hand-optimized assembler code for the core part of the solver. The performance of the calculation part is 186 MFLOPS per node, which is 62% of the peak speed. The percentage of the communication in the total is 23 %, which makes the sustained speed for the solver 148 MFLOPS. This is about a half of the theoretical peak speed.

We also measured the performance of the LINPACK benchmark. The sustained speed for the case of 2048 PU's is 368.2 GFLOPS, which is 59.9% of the theoretical peak speed. This performance was ranked as number one of TOP 500 Supercomputers announced in November 1996.

§5. Physics Results

5.1. Hadron Spectrum in Quenched QCD

Deriving the hadron spectrum from lattice QCD is a milestone to verify that QCD is the fundamental theory of quarks and gluons. Therefore, much effort has been paid to calculate the hadron spectrum⁶⁾ since 1981 when the first attempt of the hadron spectrum calculation was made⁷⁾.

A simulation of QCD without approximation requires an enormous computer time. Therefore, as the first step, the quenched approximation, in which pair creations and annihilations of quarks in the vacuum are ignored, has been employed in major simulations of QCD. However, even in the quenched approximation, it is not easy to obtain precise values of the hadron spectrum. We have to first control and then estimate various systematic errors characteristic of lattice QCD, i.e., the errors due to the infinite volume limit and the continuum limit. Moreover, it is technically difficult to simulate directly at the realistic values of light u and d quark masses, as the CPU time is proportional to the inverse of the quark mass. Therefore we have to extrapolate results obtained at relatively heavy quark masses to the light quark mass. This introduces another source of systematic errors.

In early works, it was difficult to employ large enough lattices with small enough lattice spacings, mainly due to limitation of computer power. In particular, all simulations before 1988 employed lattices much smaller than 2 fm which is the size of typical hadrons. Therefore old calculations suffer from large systematic errors. Simulations at light enough quark mass were also difficult due to algorithm adopted and the speed of computers at that time.

The best calculation prior to the CP-PACS was performed by the GF11 collaboration⁸⁾ in 1992-1993 using their dedicated computer GF11. Performing systematic extrapolations in terms of quark masses and lattice spacing, supplemented by corrections from the finite lattice size, they determined the quenched hadron spectrum in the continuum limit. They concluded that the hadron masses in the quenched QCD are consistent with experiment within their errors, which is typically about 10%.

As the first physics project on the CP-PACS, we aimed to obtain final results for the hadron spectrum in the quenched QCD with errors of a few % level and thereby clarify the long standing issue of the magnitude of quenching errors. Simulation parameters were chosen by taking this goal into consideration.

From these simulations together with detailed systematic analyses, we succeed to determine the quenched hadron spectrum with errors about 1-2 % for mesons and 2-3 % for baryons⁹⁾. We were also able to much reduce various systematic errors and estimate them. This is crucial to obtain reliable numerical results. Thus we are able to establish the hadron spectrum in the quenched QCD.

In Fig.2, our results for the quenched spectrum together with experiment are shown. The experimental values of the π , ρ and K or ϕ masses are employed to fix the physical scale and the light quark masses.

Our results unambiguously establish a discrepancy between the quenched hadron masses and the experimental values, with up to 7σ for several particles. On the

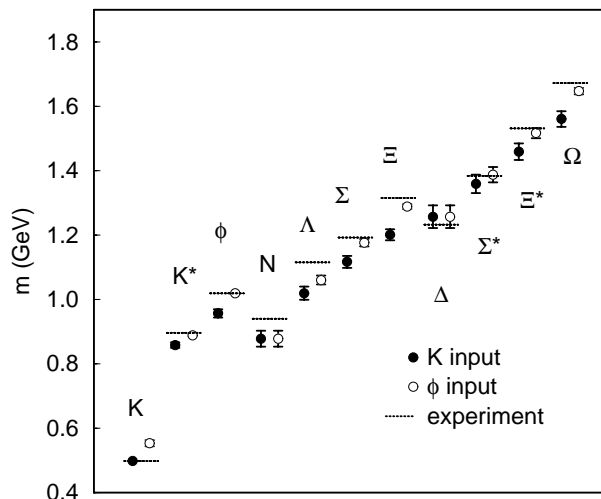


Fig. 2. Hadron masses in quenched QCD, compared with experiment.

other hand, the magnitude of the discrepancy is at most 10%, which is consistent with phenomenological estimates of the quenching error.

5.2. Hadron Spectrum in Full QCD

Since the quenched hadron mass spectrum exhibits deviation from experiment, the next step is to perform calculation of QCD without the quenched approximation (the full QCD calculation). As a step toward this goal, we have started QCD simulations taking into account of effects of pair creation and annihilation of light u , d quarks. We treat the heavier s quark in the quenched approximation.

Simulations in full QCD need computer power at least 100 times larger than that in the quenched QCD. Therefore, it is impossible to simply repeat the simulation in full QCD like that described above in the quenched QCD. In order to overcome this problem, we adopt an improved action, which is a lattice action modified in such a way that systematic errors due to finite lattice spacing is reduced.

We first made a pilot study to investigate the effects of improving using various improved actions and found that the combination of the renormalization-group improved action¹⁰⁾ for gluons and the clover action¹¹⁾ significantly reduces errors due to the finite lattice discretization over the standard action¹²⁾. We adopt this combination of improved actions in our production runs.

A systematic study of the mass spectrum in full QCD is in progress. We have already found several interesting effects of dynamical quarks in the hadron spectrum. In Fig.3 we compare meson masses in full QCD with those in the quenched QCD. It clearly shows that in the continuum limit (the point where the lattice spacing a is zero) the discrepancies of K^* and ϕ meson masses from experiment observed in the quenched QCD are significantly reduced in full QCD¹³⁾.

5.3. Quark Masses

The masses of quarks are the very fundamental parameters in nature like the mass of the electron. However, because quarks are confined in hadrons, one cannot

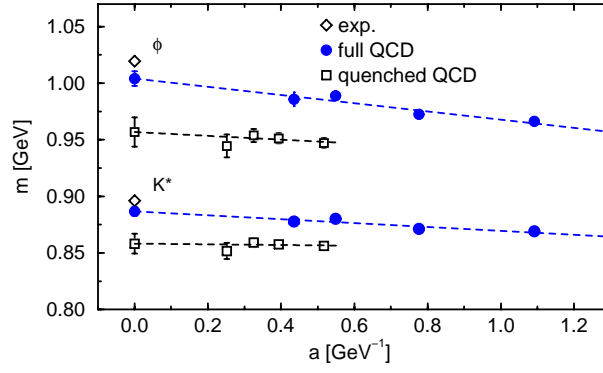


Fig. 3. Meson masses in full QCD compared with those in quenched QCD; their lattice spacing dependence and continuum limits.

determine their masses directly from experiment. Usually, their values have been theoretically inferred from experimental hadron masses using phenomenological models of QCD. Lattice QCD is the only known way to determine the masses of quarks from first principles.

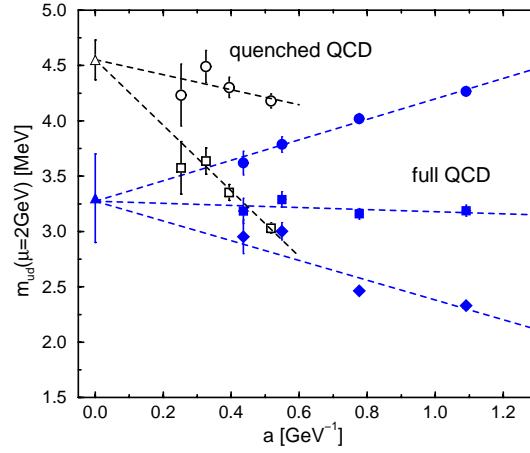


Fig. 4. Mass of the average of u and d quarks; lattice spacing dependence and continuum limit.

We made systematic calculations of quark masses both in the quenched QCD and in full QCD¹³⁾. In Figs. 4 and 5 we show the lattice spacing dependence of the average u , d quark mass and the s quark mass, respectively.

On the lattice there are alternative definitions of the quark mass. Although the values of the quark mass differ depending on the definition at finite lattice spacing, they extrapolate to a common value in the continuum limit. The verification of the unique value in the continuum was first made in the quenched QCD in Ref.14). This verification is important because the quark mass should be the fundamental parameter in QCD.

The s quark mass is determined using experimental values of either K meson mass or ϕ meson mass. The s quark mass in the quenched approximation depends on the choice of input. This reflects a systematic error of quenching.

The discrepancy is found to be much reduced in our full QCD calculations. The

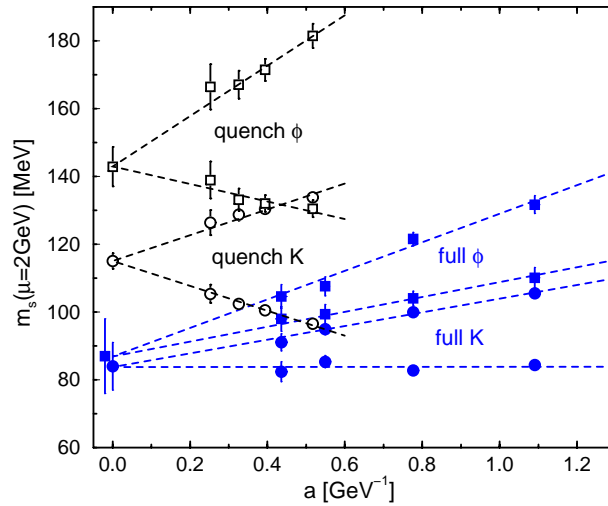


Fig. 5. Mass of the s quark; lattice spacing dependence and continuum limit.

values of the s quark mass from K meson mass or ϕ meson mass are consistent within one standard deviation; 90(10) MeV. This value is significantly smaller than that in the quenched QCD; 120-140 MeV. The value 90(10) MeV for the s quark mass has a significant implication for the analysis of the CP violation.

For the clarification of the CP violation in nature we need a theory like the Kobayashi-Maskawa theory, an experiment result like that from a B factory, and also numerical results from lattice QCD. This is a typical example of cases where results from three fields of theoretical physics, experimental physics and computational physics are necessary to solve a problem.

§6. Conclusions

It was successful to develop a massively parallel computer CP-PACS with a peak speed of 614 GFLOPS due to a close collaboration among physicists, computer scientists and a vendor. The performance of the computer for physics application is as high as 50 % of the peak speed in the case of the core part of lattice QCD programs.

We are able to obtain interesting and important results in lattice QCD using the CP-PACS computer: 1) The hadron spectrum in the quenched QCD has been established. Our results unambiguously clarify a discrepancy between the quenched hadron masses and the experimental values, with up to 7σ for several particles. On the other hand, the magnitude of the discrepancy is at most 10%, which is consistent with phenomenological estimates of the quenching error. 2) The discrepancies of meson masses from experiment observed in the quenched QCD are significantly reduced in full QCD. 3) We have systematically calculate the masses of light quarks in the quenched QCD and in full QCD. In particular, the mass of the s quark in full QCD is 90(10) MeV, which is much smaller than that previously estimated phenomenologically.

ACKNOWLEDGEMENTS

I would like to thank the members of the CP-PACS Project and the members of the CP-PACS Collaboration for lattice QCD simulations, in particular, K. Nakazawa and A. Ukawa for valuable discussions. This work is supported in part by the Grand-in-Aid of the Ministry of Education, Science and Culture (Nos. 08NP0101 and 09304029).

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